**Title:** **Exploratory Research on Simulation of CO$_2$-Brine-Mineral Interactions**

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Grant Number            DE-FG26-03NT41806
Performance Period      September 1, 2003 – August 2005

## 1. Abstract

**- OBJECTIVE(s)**

Application of many carbon sequestration strategies requires knowledge of thermodynamic properties for extremely complex chemical systems such as, CO$_2$-SO$_2$-H$_2$O-NaCl-CaCl$_2$-MgCl$_2$. The objective of this research is to explore a unique approach to develop a unified equation of state (EOS) to describe thermodynamic properties in the above chemical system. We started the research project by assessing the currently available data and models, and their appropriateness for the carbon sequestration process. We have then worked on the building blocks for the unified model. CO$_2$ solubility models for the CO$_2$-H$_2$O-NaCl system has been updated with newly available experimental data and based on the new development in thermodynamics and molecular dynamics. This will allow computer simulations of geochemical reactions in laboratory experiments and permit upscaling to industrial and field-scale production. A strategy to address the complexity of the chemical system will be developed and this will help to meet the long-term goal of developing an EOS that is suitable for the temperature

**- ACCOMPLISHMENTS TO DATE**
The project was delayed because Chen Zhu has moved to Indiana University. However, in the past year, we have reviewed literature data on the thermodynamic properties in the systems CO$_2$-H$_2$O and CO$_2$-H$_2$O-NaCl. From this literature review, we have identified the experimental data needs. We have also modified and updated the CO2 solubility model, which will allow efficient calculations in large scale numerical simulation (e.g., reservoir and basin scale) and also is updated to reflect newly available experimental data.

**- FUTURE WORK**
Complete the project by the end of summer 2005 and submit the report.

**- LIST OF PAPER PUBLISHED, U.S. PATENT/PATENT APPLICATION(S),**
     **CONFERENCE PRESENTATIONS, STUDENTS SUPPORTED UNDER THIS**
     **GRANT**

Two papers are at the preparation stage:

"PVTx Properties of the CO2-H2O and CO2-H2O-NaCl Systems: Assessment of experimental data and thermodynamic models"

" An improved model for the calculation of CO2 solubility in aqueous solutions"

A graduate student Mathew Reeder has been supported by this grant.